Ethanol 64-17-5 | DTXSID9020584

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.05

Global applicability domain: Inside

Local applicability domain index: 9.28e-01

Confidence level: 5.68e-01

Nearest Neighbors from the Training Set

Image not found

Ethanol Measured: 3.25 Predicted: 3.05 Image not found

Acetic acid
Measured: 4.31
Predicted: 3.69

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Isopropanol
Measured: 3.41
Predicted: 3.68

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Dimethylamine Measured: 2.00 Predicted: 2.62 Image not found

Methylamine
Measured: 1.90
Predicted: 2.59